

# Hartree-Fock for nuclei

## Key concepts:

- HO basis provides good starting point  
→ especially spherical nuclei
- Standard shell model ordering to charge occupied states
- Many-body Hamiltonian includes kinetic energy  $T$ , two-body interactions  $V_{NN}$ , three-body interactions  $V_{3N}$
- Hartree-Fock will give us an optimized basis, but limited by basis truncation parameters

## Basis states, spherical harmonic oscillator

Choose 1-body basis  $|p\rangle$  as eigenstates of spherical HO:

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} r^2$$

**HO frequency** sets (inverse) "width" of oscillator potential

→ should not be too far away from size of nucleus

HO states

$$|n_x n_y n_z\rangle = |n l m\rangle = |p\rangle$$

$$n = 0, 1, 2, \dots$$

$$l = 0, 1, 2, \dots$$

$$m = -l, -l+1, \dots, l$$

Useful: HO energy number  $E = 2n + l$

$\Rightarrow$  energy of  $|nlm\rangle$  is  $(E + \frac{1}{2})\hbar\omega$

$\Rightarrow$  HO energy number  $E$  allows one to organize basis

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$E=3$

$\overline{n=1, l=1}$

$\overline{n=0, l=3}$

$E=2$

$\overline{l=0, n=1}$

$\overline{l=2, n=0}$

$E=1$

$\overline{n=0 \quad l=1}$

$E=0$

      

allowed states only  $n=0, l=0$

Naming Scheme:

s:  $l=0$

d:  $l=2$

p:  $l=1$

f:  $l=3$

Final step couple to total angular momentum  $\vec{J} = \vec{L} + \vec{S}$

why?

- nucleons are spin  $1/2$
- nature is rotationally invariant

$\Rightarrow J$  is a good quantum number of physical states

$$|nlsm_s m_e\rangle \rightarrow |n(ls)jm_j\rangle$$

$$= \sum_{m_s m_e} C_{l m_e s m_s}^{j m_j} |nlsm_s m_e\rangle$$

Clebsch-Gordan coefficient

$\Rightarrow$  add iso spin  $m_t = \frac{1}{2}$  (proton)  
 $-\frac{1}{2}$  (neutron)

$|n(ls)jm_j m_t\rangle$  = single-particle basis

Notation:  $0s\frac{1}{2} = n=0 \quad l=0 \quad j=\frac{1}{2}$

# H<sub>0</sub>      H<sub>0</sub> + spin-orbit

$e = 3$



of $5/2$	6
1P $1/2$	2
1P $3/2$	4
of $7/2$	8

$e = 2$

20	od $3/2$	4
	1s $1/2$	2
	od $5/2$	6

$e = 1$

	op $3/2$	2
	op $5/2$	4

$e = 0$

2	os $1/2$	2
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$\Rightarrow$  (2), (8), (20) are "magic"

numbers  $\Rightarrow$  especially deeply bound

Use this ordering to determine occupied levels

Q: What about  $m_j$ ?

- Basis ✓

→ Next: Hamiltonian

$$H = T + V_{NN} + V_{3N}$$

Problem:  $\bar{T}$  is total kinetic energy  
including center of mass ( $C.M.$ )

→ But binding energy does not depend  
on C.M. kinetic energy

Solution:

subtract C.M. kinetic energy

$$T_{cm} = \frac{1}{2A^m} \left( \sum_i \vec{p}_i \right)^2$$

Our Hamiltonian is  $A$ -dependent due  
to C.M. correction

$$H = T - T_{cm}(A) + V_{NN} + V_{3N}$$

What we have:

$$T_{pq}(\hbar\omega) \quad T_{cm, pqrs}(\hbar\omega) \quad U_{NN, pqrs}(\hbar\omega)$$



$T_{cm}$  is a 1+2-body operator

$\Rightarrow V_{3N, pqrs t u}$  after lunch



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Final considerations:

— Basis size will be finite

example: include all states with

$$e \leq e_{max} = 4$$

— Basis depends also on  $\hbar\omega$  (HO width)

— Q: How do we choose  $e_{max}, \hbar\omega$ ?

$\Rightarrow$  Vary and check convergence

—  $e_{max} \rightarrow e_{max+1}$  does not change?

- trw behavior can be optimized using variational principle

